

Realization of a “Two Relaxation Rates” in the Hubbard-Falicov-Kimball Model

H. Barman^{1,*}, M. S. Laad^{1,†}, and S. R. Hassan^{1,‡}

¹*Institute of Mathematical Sciences, Taramani, Chennai 600113, India*

A single transport relaxation rate governs the decay of both, longitudinal and Hall currents in Landau Fermi Liquids (LFL). Breakdown of this fundamental feature, first observed in cuprates and subsequently in other *three-dimensional* correlated systems close to (partial or complete) Mott metal-insulator transitions, played a pivotal role in emergence of a non-Landau Fermi liquid paradigm in higher dimensions $D(> 1)$. Motivated hereby, we explore the emergence of this “two relaxation rates” scenario in the Hubbard-Falicov-Kimball model (HFKM) using the dynamical mean-field theory (DMFT). Specializing to $D = 3$, we find, beyond a critical FK interaction, that two distinct relaxation rates governing distinct temperature (T) dependence of the longitudinal and Hall currents naturally emerges in the non-LFL metal. We rationalize this surprising finding by an analytical analysis of the structure of charge and spin correlations in the underlying impurity problem, and point out good accord with observations in the famed case of $V_{2-y}O_3$ near the MIT.

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It is well known that a single transport relaxation rate governs the decay of both longitudinal and Hall currents in a Landau Fermi liquid (LFL) metal. This is obviously related to the fact that both result from scattering processes involving the same Landau quasiparticle, carrying the quantum numbers of an electron. Observation of distinct relaxation rates in dc resistivity (ρ_{dc}) and Hall angle (θ_H)¹ data for cuprates led to a paradigm shift in the traditional view of strongly correlated electrons in metals in dimension $D > 1$. While such anomalous behavior can be rationalized in $D = 1$ Luttinger liquids (LL) by appealing to fractionalization of an electron into a neutral spinon and a spinless holon, the specific nature of electronic processes leading to emergence of such features in $D > 1$ is an enigma. In fact, Anderson² *predicted* such a feature from a generalized “tomographic” LL state in $D = 2$, by hypothesizing spin-charge separation: $\rho_{dc}(T) \simeq T$ arose from holon-spinon scattering, while $\cot\theta_H(T) \simeq T^2$ emerged from spinon-spinon scattering. Though very attractive, a derivation of such a higher- $D = 2$ LL-like state remains an open and unsolved issue of great current interest.

Surprisingly, subsequent experiments revealed similar “two relaxation rates” in $D = 3$ correlated systems as well. Specifically, simultaneous resistivity and Hall measurements in the classic Mott system $V_{2-y}O_3$ ³ revealed the following: in the lightly doped ($0 < y \ll 1$) case, (i) the dc resistivity, $\rho_{dc}(T) = \rho_0(y) + A(y)T^{1+\eta(y)}$, with $\eta(y) \leq 1.5$, while the Hall angle, $\cot\theta_H(T) \simeq C_1 + C_2T^2$, independent of y for all $T > T_N(y)$, the Néel ordering temperature. This is the first known example of a $D = 3$ correlated metallic system exhibiting “two” relaxation rates, and similar behavior is also seen in nearly cubic $CaRuO_3$ ⁴ and $YbRh_2Si_2$ ⁵. These observations show that such novel features are not unique to $D = 2$ systems, but generic to metallic states on the border of the Mott MIT. It is also interesting⁶ that disorder seems to be a very relevant perturbation in $V_{2-y}O_3$: the resistivity is well accounted for by a variable-range hopping form, attesting to importance of disorder near the Mott tran-

sition. In multi-orbital $CaRuO_3$ and $YbRh_2Si_2$, orbital-selective physics^{4,7} generically leads to extinction of LFL metallicity via “Kondo breakdown” and onset of “spin freezing”, wherein one would expect low-energy charge dynamics to be controlled by the (strong) “intrinsic disorder” scattering between the quasi-itinerant and effectively Mott localized components of the full one-particle spectral function (though, strictly speaking, consideration of $YbRh_2Si_2$ would require a multi-band periodic Anderson model). The actual Mott transition in V_2O_3 is by now also established to involve multi-orbital correlations and orbital-selective localization: in LDA+DMFT studies⁸⁻¹⁰, the e_g^π states remain Mott localized, while the a_{1g} states remain bad-metallic in the bad-metal close to the MIT. In the quantum paramagnetic state where the Mott transition occurs, one may view the e_g^π states as providing an “intrinsic disorder”, providing a strong scattering channel for the a_{1g} carriers. Thus, it seems that the anomalous two-relaxation times are linked to the breakdown of LFL metallicity arising from strong scattering processes involving either intrinsic scattering channels or extrinsic disorder close to the MIT.

Motivated by these observations, we introduce a Hubbard-Falicov-Kimball model in standard notations

$$H_{\text{HFKM}} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h. c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + U_{cd} \sum_{i,\sigma} n_{ic\sigma} n_{id} \quad (1)$$

as an *effective* model that captures the interplay between itinerancy (t) and strong electronic correlations (U) and intrinsic or extrinsic (U_{cd}) disorder scattering. Qualitatively, (i) U_{cd} can mimic an effectively Mott-localized band in an orbital-selective Mott transition (OSMT) scenario, or (ii) $v_i = U_{cd} n_{id}$ can also be viewed as an extrinsic disorder potential experienced by the correlated c -fermions (in $V_{2-y}O_3$, one can regard this as disorder arising from a concentration y of V-vacancies in the host system). We solve H_{HFKM} using the dynamical mean-

field theory (DMFT) with iterated perturbation theory (IPT) as the solver for the effective impurity problem¹¹. In our method, U_{cd} is treated as site-diagonal disorder within coherent potential approximation (CPA)¹² using a semi-circular band density of states for the c -electrons as an approximation to the actual $D = 3$ system (it keeps the correct energy dependence near the band edges in $D = 3$). Within DMFT, it is long known that a correlated LFL metal for small U_{cd} smoothly goes over to an incoherent bad metal without LFL quasiparticles as U_{cd} increases. Motivated by the fact that two-relaxation times seem to be linked to proximity to the (pure or selective) Mott transition, we focus on the evolution of the (magneto)-transport when U_{cd} is cranked up in the regime where $U/t = 3.3$ is chosen to be close to the critical $(U/t)_c \simeq 3.4$ where a purely correlation-driven Mott transition¹³ obtains. Since the relevant DMFT formalism and the associated equations have already been discussed in Ref. 12 in the related context of a binary-alloy disordered Hubbard model (the same IPT+CPA also solves the HFKM *exactly* in DMFT for the c_σ -fermions), we do not repeat them here.

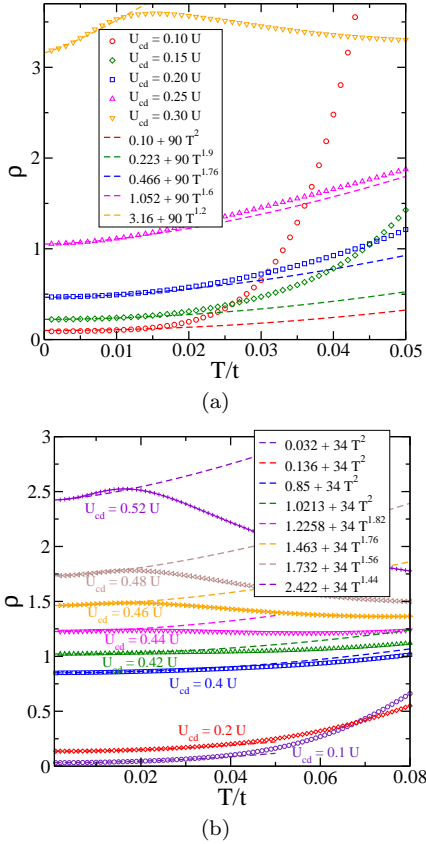


FIG. 1. DC resistivity vs temperature plot at (a) $U = 3.3t$ and (b) $U = 2.0t$. Dashed lines are power-law fits at low T .

In Fig. 1, we exhibit the dc resistivity, $\rho_{dc}(T, U_{cd})$ for different U_{cd} and fixed $U/t = 3.3$ as a function of T . Several features stand out clearly: a correlated LFL up to small $U_{cd} < 0.2U$, where $\rho_{dc} = \rho_0(U_{cd}) + A(U_{cd})T^2$,

smoothly evolves into an incoherent metal for $U_{cd} = 0.2U$, where we find $\rho_{dc}(T) = \rho_0 + A_1 T^\alpha$, with $\alpha = 1.76$. It is very interesting that α seems to vary continuously with U_{cd} , ($\alpha = 1.6$ for $U_{cd} = 0.25U$, $\alpha = 1.2$ for $U_{cd} = 0.3U$), and the fact that ρ_{dc} remains bad-metallic at intermediate-to-low T , crossing over to an insulator-like form at high T for $U_{cd} = 0.3U$. Repeating the calculations for smaller $U/t = 2.0$, we find that while qualitatively similar features obtain, $\rho_{dc}(T \rightarrow 0)$ rises to much higher values when U_{cd} is cranked up. This testifies to the increasing relevance of the strong scattering (from localized channels or extrinsic disorder as above) when U/t is in the weak-to-intermediate coupling regime. Since transport properties in DMFT do not involve vertex corrections in the Bethe-Salpeter equations for the conductivities, these features must be tied to loss of the LFL quasiparticle pole structure in the DMFT one-electron propagator, which is now the sole input to the renormalized bubble diagram for the conductivities¹³.

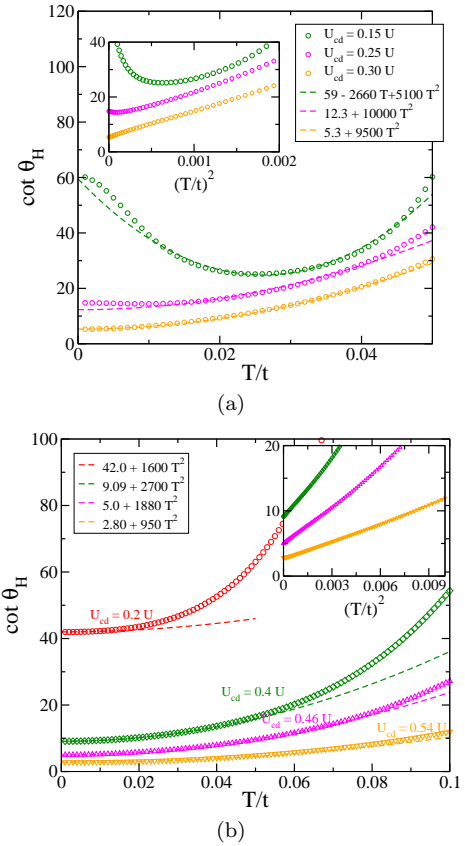


FIG. 2. Cotangent of Hall angle (θ_H) vs temperature plot at (a) $U = 3.3t$ and (b) $U = 2.0t$. Dashed lines are power-law fits at low T . Insets show the same against T^2 .

Upon evaluating the off-diagonal conductivity (to first order in the vector potential \mathbf{A} as done before¹⁴) for H_{HFKM} in DMFT, we have computed the Hall constant (R_H) and Hall angle ($\cot \theta_H$) for the same parameter values as above. Even more remarkably, we find (see Fig. 2) that $\cot \theta_H \simeq C_1 + C_2 T^2$, up to $T/t = 0.05$

for both $U_{cd}/U = 0.25, 0.3$, while R_H exhibits a strong T -dependence right down to the lowest T (see Fig. 3). This is the *same* parameter regime where $\rho_{dc}(T)$ exhibits non-LFL T -dependence, with a U_{cd} -dependent exponent $1.0 < \alpha < 2.0$. Thus, our DMFT results directly reveal two-relaxation rates, and it is indeed notable that $\cot\theta_H \simeq C_1 + C_2 T^2$ continues to hold over a wide T range, even as the exponent α continuously varies between 1.0 and 2.0. Our results are completely consistent with data for $V_{2-y}O_3$ ³ in all respects: (i) specifically, $\rho_{dc}(T) \simeq \rho_0(y) + AT^\alpha$ with $1.3 \leq \alpha \leq 1.5$ in data agrees well with our estimate $1.2 \leq 1.76$ in the non-LFL regime of H_{HFKM} , (ii) $\cot\theta_H(T) = C_1 + C_2 T^2$ up to $T \simeq 500$ K upon choosing $t = 1.0$ eV in the model, again in nice accord with data. Moreover, $\cot\theta_H$ also exhibits an upward curvature at very low T in DMFT, again in complete accord with data. (iii) Concomitantly, $R_H(T)$ exhibits a strong T -dependence, increasing with decreasing T before peaking at very low T before AF order occurs at $T \simeq 10$ K.

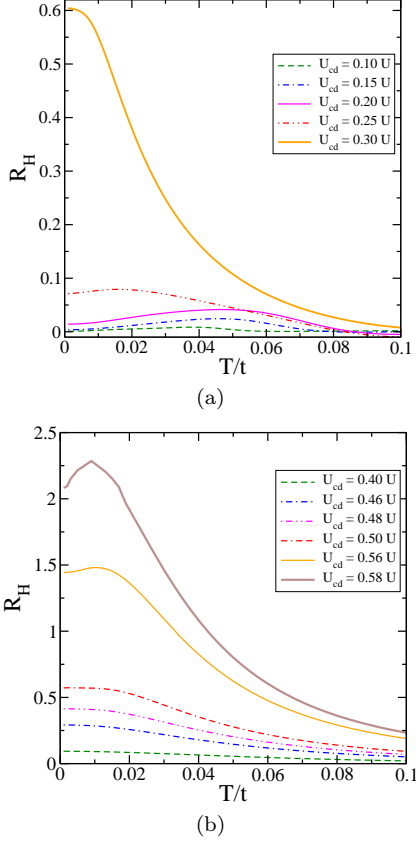


FIG. 3. Hall coefficient (R_H) vs temperature plot at (a) $U = 3.3t$ and (b) $U = 2.0t$. Dashed lines are power-law fits at low T .

Thus, (magneto)transport responses in H_{HFKM} within DMFT exhibit comprehensive qualitative accord with the complete set of data for $V_{2-y}O_3$. In particular, our results now strongly support the notion that emergence of two relaxation rates, or that the different decay rates for

longitudinal and Hall currents, is a direct consequence of breakdown of the LFL metal by strong scattering. As discussed above, the FK term in Eq.(1) can mimic either “intrinsic” scattering coming from selectively Mott localized states in a multi-band system, or arising from strong “disorder” scattering. Indeed, singular behavior of the γ -coefficient of the specific heat¹⁵ has also been recently found in a binary-alloy Hubbard model: we emphasize that this is isomorphic to our HFKM, since the FK term can also be interpreted as a binary alloy disorder term in the Hubbard model. Thus, a similar divergence of $\gamma(T) = C_{\text{el}}(T)/T$ will also appear in our HFKM within DMFT. This generic effect of a strong intrinsic (or extrinsic, of the binary-alloy disorder type) will be generally relevant close to a correlation-driven MIT. This is because correlations have already drastically renormalized the band energy scale to a much lower value associated with collective Kondo screening induced “heavy” LFL. In such a situation, even modest disorder will appear “strong”, since the relevant scale that sets the relevance of disorder is now $(U_{cd}n_{id}/k_B T_{\text{coh}})$ (with coherence temperature T_{coh} being small near the Mott transition) rather than $(U_{cd}n_{id}/W)$, with W the free bandwidth for $U = 0$.

These observations call for a deeper understanding in terms of basic microscopic responses involving interplay between the FK term and Mottness. Since DMFT is a self-consistently embedded impurity problem, and the anomalies are seen in the strongly correlated metallic state, we choose to tease out the deeper underlying reasons by analyzing the “impurity” model. In analogy with DMFT studies for the Hubbard model, the appropriate impurity model is the Wolff model of a correlated d -impurity coupled to a bath of “conduction” electrons, as well as to a localized scattering potential (U_{cd}). We find it most convenient to bosonize this impurity model by generalizing earlier attempts¹⁶. Such an analysis has the potential to bare the asymptotic separation of spin- and charge modes, facilitating DMFT observation of two relaxation rates. The Wolff impurity model including the FK coupling reads

$$H_W = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + U n_{0,d,\uparrow} n_{0,d,\downarrow} + U_{cd} \sum_{\sigma} n_{0,c,\sigma} n_{0,d} - \mu \sum_{\sigma} n_{0,c,\sigma}. \quad (2)$$

The Wolff model for $U_{cd} = 0$ is bosonized as usual on a $(1+1)D$ half-line and the result is a set of two independent gaussian models for *bosonic* spin and charge fluctuation modes emanating from the “impurity” (site 0) in each radial direction. The bosonized Hamiltonian is $H = H_c + H_s$ where

$$H_c = \frac{v_F}{2} \int dx \left[\Pi_c^2(x) + (\partial_x \phi_c)^2 \right] + \frac{(\mu + U n_0)}{\sqrt{2\pi}} [\partial_x \phi_c(0)] + \frac{U}{8\pi^2} [\partial_x \phi_c(0)]^2, \quad (3)$$

$$H_s = \frac{v_F}{2} \int dx \left[\Pi_s^2(x) + (\partial_x \phi_s)^2 \right] - \frac{U}{8\pi^2} [\partial_x \phi_s(0)]^2 \quad (4)$$

for a non-magnetic ground state, with n_0 corresponding to the occupation of non-interacting c -fermions. The spin and charge bosonic fields on the impurity are $\rho_s(0) = (\partial_x \phi_s)/\sqrt{2\pi}$ and $\rho_c(0) = (\partial_x \phi_c)/\sqrt{2\pi}$. v_F is the (common) Fermi velocity when $U_{cd} = 0$. The FK term couples solely to the charge bosons, but with a subtlety which will result in interesting anomalies. Viewed at the basic scattering level, $U_{cd} \sum_i n_{ic} n_{id}$ acts as a strong scattering potential. Since $[n_{id}, H] = 0 \forall i$ in the HFKM, $n_{id} = 0, 1$ and, viewed by a propagating c -fermion, $v_i = U_{cd} n_{id}$ now represents a “suddenly switched on” scattering potential that successively switches suddenly between 0 and U_{cd} . In the local impurity problem, this is thus precisely the famed “X-ray edge” (XRE) problem (U_{cd} is the precise analog of the suddenly switched-on “core-hole” potential) in the *charge* channel: the spin channel is left unaffected. In their seminal works, Anderson¹⁷ and Noziers *et al.*¹⁸ found vanishing overlap between ground states with $U_{cd} = 0$ and $U_{cd} \neq 0$, and emergence of infra-red branch-cut features in one- and two-particle propagators. Fortunately, the XRE problem is also readily amenable¹⁹ to bosonization: the crucial effect of U_{cd} is to induce a “shift” in the charge bosons. Explicitly, expanding the charge-bosonic field in Fourier components, $\phi_c(x) = \sum_k (\sqrt{2|k|})^{-1} (a_k e^{ikx} + a_k^\dagger e^{-ikx}) e^{-\alpha|k|/2}$ and $\Pi_c(x) = -i \sum_k \sqrt{|k|/2} (a_k e^{ikx} - a_k^\dagger e^{-ikx}) e^{-\alpha|k|/2}$, one gets

$$H_c = \sum_{k>0} \omega_k a_k^\dagger a_k + \frac{iv\sqrt{2\rho}}{\sqrt{N}} \sum_{k>0} (a_k - a_{-k}) - \frac{U\rho}{2} \sum_{k,k'>0} (a_k - a_{-k})(a_{k'} - a_{-k'}) \quad (5)$$

where $a_k^\dagger = a_{-k}$, we have set $\mu = U(1 - n_0)$ using Luttinger’s theorem, and work within the restricted Hilbert space where the $b_k, b_{k'}^\dagger$ satisfy Bose commutation relations. H_c now corresponds to a shifted oscillator, and the effect of U_{cd} is to generate an unrenormalizable s -wave phase shift, $\delta = \tan^{-1}(U_{cd}/2z_{\text{FL}}t)$, with z_{FL} the quasiparticle renormalization in the disorder free (pure Hubbard) model.

H_c is now a “small polaron” model with coupling between bosons at different k along different directions from the impurity, where the “polarons” are now associated with low-energy particle-hole modes. Since it is quadratic in the bosons, it can be readily diagonalized as follows: (i) the first “small polaron” like term is

transformed away by a Lang-Firsov unitary transformation, resulting in a shifted “oscillator” form¹⁹, resulting in $H_c = \sum_{k>0} (k/\rho) (a_k^\dagger + U_{cd}/\sqrt{kN})(a_k + U_{cd}/\sqrt{kN})$ and (ii) the last term, quadratic in bosons but with mixing terms such as $a_k^\dagger a_{k'}$ and $a_{k'} a_k$, simply rotates H_c to a new quadratic Hamiltonian in bosons. However, the crucial effect of the last step is to change the velocity of the charge bosons (the sole but crucial effect of U_{cd} is, via action of the term $(a_k - a_{-k}) = (a_k + a_k^\dagger)$, to “distort” the Luttinger Fermi sea for the charge, but *not* for spin): thus, this results in different velocities for charge and spin modes, with $v_c > v_s$. The charge-bosonic propagator will acquire an anomalous dimension, while the spin-fluctuation propagator will retain its “Fermi liquid” like character. Put another way, the charge fluctuation propagator now has a branch-cut, but the spin fluctuation propagator retains its infra-red pole structure. Upon refermionization of H_s (note that this *cannot* be done for H_c in view of the orthogonality catastrophe), we find that the spin excitations are expressible as *fermions*: following Anderson, one may call them “spinons”. Remarkably, this bears close similarity to Anderson’s hidden-FL²², and the above can be viewed as a high-dimensional spin-charge separation.

An external electric field accelerates charge, leading to a spinon backflow and induces scattering between spin and charge. In $D = 3$, one expects that scattering off local, dynamical spin fluctuations will lead to the dc resistivity $\rho_{\text{dc}}(T) \simeq T^{D/2} = T^{3/2}$. However, an external magnetic field will couple solely to the spin modes (equivalently spin-fermions or “spinons” as above), leading to a Hall relaxation rate entirely determined by “spinon-spinon” scattering, giving $\cot\theta_H \simeq \tau_H^{-1} = C_2 T^2$. In presence additional strong scattering due to either an intrinsically localized electronic (U_{cd}) or disorder channel, there will generically be a term $\tau_H^{-1} \simeq C_1$ in addition to the above, yielding $\cot\theta_H \simeq C_1 + C_2 T^2$. On the other hand, since the charge fluctuations are directly affected thereby, the resulting modification of scattering processes involving charge and spin modes can lead to deviation from the $\rho_{\text{dc}}(T) \simeq T^{3/2}$ in addition to contributing a residual ρ_0 term.

The finding of two relaxation rates for decay of longitudinal and Hall currents can now be rationalized by observing that these are consequences of breakdown of LFL concepts in the barely (bad) metallic state close to the Mott transition. Extinction of LFL quasiparticles is associated with a “lattice” orthogonality catastrophe, which now occurs due to either U_{cd} ²⁰ or strong disorder²¹ in a metal already close to a correlation-driven Mott transition. In this context, it is interesting to observe that the hidden-FL²² also involves a related X-ray-edge mechanism (at $U = \infty$) for destruction of LFL theory. In our case, given finite $U \simeq W$ (the one-electron bandwidth), additional intrinsic (U_{cd}) or extrinsic (disorder) scattering channels are necessary to generate such breakdown of LFL theory. Turning to $D = 2$, observation of similar features in near-optimally doped cuprates will require ap-

peal to cluster extensions of DMFT (which, among other things, cannot access dynamical effects of non-local spatial correlations near a Mott transition). However, our use of DMFT is known to be a reliable approximation for $D = 3$.

To summarize, we have investigated emergence of two relaxation rates in correlated metals close to the Mott transition in $D = 3$. We find that this unique feature is tied to loss of LFL metallicity in symmetry-unbroken metallic states proximate to Mott transition(s): this can arise from strong scattering processes either stemming from intrinsic, (selectively-Mott) localized electrons, or from disorder which is generically relevant near a MIT.

It is thus not specific to $D = 2$. Surprisingly, comparison with data³ for $V_{2-y}O_3$ reveals very good qualitative accord with all unusual features: (i) $\rho_{dc} \simeq \rho_0(y) + AT^{\alpha(y)}$ with $1.2 \leq \alpha \leq 1.6$, (ii) a strong T -dependent Hall constant, peaking at low T , and (iii) much more disorder-independent behavior of $\cot\theta_H(T) \simeq C_1 + C_2T^2$.

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* hbarhbar@gmail.com

† mslaad@imsc.res.in

‡ shassan@imsc.res.in

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